Constrained Interpolation Remap of Discrete Divergence Free Fields

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We present a constrained interpolation (CI) algorithm for remapping of divergence free vector fields encoded as 2-cochains on a two-dimensional cell complex. On contractible domains discrete divergence free fields are 2-coboundaries and so they have potentials represented by 1-cochains. The algorithm takes advantage of this fact by using the discrete potential to effect the remapping of the divergence free field. The discrete potential is reconstructed and interpolated to the new cell complex. Application of the coboundary operator gives the discrete divergence free field on the new mesh. In contrast to advection-based remappers, this algorithm has several valuable advantages. The new cells are not required to be small perturbations of the old cells. The grids can have different connectivities and can consist of different cell types. The CI algorithm also avoids the complications arising from the need to upwind on unstructured grids in transport-based remappers.

Introduction

Transfer of data between different grids, subject to constraints, is fundamental to many numerical algorithms. An important example is Arbitrary Lagrangian-Eulerian (ALE) methods, which combine a Lagrangian update with rezoning to reduce grid distortion and remapping to transfer solution to the rezoned mesh. A computational strategy that can combine the best properties of Eulerian and Lagrangian methods is to execute rezoning and remapping at every time cycle. The accuracy of such continuous rezone ALE strongly depends on the availability of efficient and accurate remappers. For instance, remapping of concentrations or density fields must preserve positivity and total mass (Margolin and Shashkov, 2003), while a magnetic flux **B** must remain divergence-free; see (Brackbill and Barnes, 1980) for the importance of this constraint in MHD.

In a continuous rezone ALE method individual cell movements are limited to small perturbations. As a result, remappers have been defined by using advection algorithms (Evans and Hawley, 1988). However, connection between the advection equation and remapping of discrete divergence free vector fields does not appear to be well understood, in particular, the discretization errors in advection remappers are not easily identified.

Alternatively, we can view remapping of divergence free fields as an interpolation procedure that may be additionally constrained to provide physical solutions (Margolin and Shashkov, 2003). Interpretation of remap as interpolation rather than as advection is more flexible because it allows formulation of algorithms on arbitrary pairs of grids and circumvents the need for upwinding on unstructured grids.

In this paper we present a constrained interpolation remap algorithm for divergence-free vector fields, represented by 2-cochains on a cell complex, without reference to advection. Given a 2-cochain b with the property that $\delta b=0$, where δ is the coboundary, the algorithm starts with an explicit recovery of a 1-cochain a with the property that $\delta a=b$. This recovery is made possible by the exactness property of the cochain complex (Bochev and Hyman, 2005). Post-processing is used to increase the order of the recovered potential and local optimization is used to determine a convex combination of high and low order potentials that minimizes the energy difference between the original and the remapped cochains. The optimized potential is interpolated to the new cell complex where application of δ gives the remapped discrete divergence free field. Because our algorithm is formulated for cochains it can be easily extended to a large class of mimetic discretizations, that use cochains to represent scalar and vector fields (Bochev and Hyman, 2005).

There are several aspects of our approach that set it apart from the existing methods. Divergence-free remappers are normally defined on Cartesian grids, using a dimension-by-dimension approach. Often they require additional restrictions, such as grid hierarchy, or factor-of-two refinement; see (Balsara, 2001), (Toth and Roe, 2001). Methods on unstructured grids usually employ Lagrange multipliers (Carey et al, 2001) and are non-local. This reduces their efficiency compared to advection remappers. In contrast, interpolation of a potential instead of using a Lagrange multiplier allows us to enforce divergence free explicitly and without solving an indefinite saddle-point system.

We formulate and present the CI remapper for cochains on a logically Cartesian cell complex. The method is illustrated by using two-dimensional cyclic remap problems. Numerical examples demonstrate attractive numerical properties of the CI remap including handling of discontinuities and energy dissipation.

Constrained Interpolation Remap

For definitions of chains, cochains, the associated boundary and coboundary operators, and how they are used to define mimetic discretizations we refer to (Bochev and Hyman, 2005). In this paper, we focus on application of the mimetic framework described in (Bochev and Hyman, 2005) to the remap problem.

Formulation of the remap problem

Let Ω denote a bounded open region in two dimensions. We assume that Ω contractible. To apply the mimetic structures of (Bochev and Hyman, 2005) it is profitable to think of Ω as a three-dimensional region obtained by extruding the original domain by a constant "thickness". The computational grid on Ω is represented by a chain complex. We assume that two such complexes, denoted by $\mathcal{K}=\left(C_0,C_1,C_2,C_3\right)$ and $\tilde{\mathcal{K}}=\left(\tilde{C}_0,\tilde{C}_1,\tilde{C}_2,\tilde{C}_3\right)$, respectively, are given on Ω. Cochains represent vector and scalar

fields. The cochain complex on $\mathcal{K}$ is denoted by $C = \left(C^0, C^1, C^2, C^3\right)$ and the complex on $\tilde{\mathcal{K}}$ - by $\tilde{C} = \left(\tilde{C}^0, \tilde{C}^1, \tilde{C}^2, \tilde{C}^3\right)$. The statement of the remap problem is as follows:

Given a 2-cochain $b \in C^2$ *on* $\mathcal{K}$*, such that* $\delta b = 0$*, find a 2-cochain* $\tilde{b} \in \tilde{C}^2$ *on* $\tilde{\mathcal{K}}$ *such that* $\delta \tilde{b} = 0$ *and* $\tilde{b} \approx b$.

The cochain $b \in C^2$ represents a divergence free field on the "old" mesh $\mathcal{K}$. In the remap problem, we seek to recover a cochain $\tilde{b} \in \tilde{C}^2$ that represents the same field on the "new" grid $\tilde{\mathcal{K}}$, by using only the information about this field encoded in $b \in C^2$. In what follows, for simplicity we assume that the chain complex is defined with respect to a logically Cartesian (but non-uniform) grid partition of Ω into quadrilateral cells.

Discrete exactness

A fundamental property of $C = \left(C^0, C^1, C^2, C^3\right)$ is the exactness

$$0 \to C^0 \xrightarrow{\delta} C^1 \xrightarrow{\delta} C^2 \xrightarrow{\delta} C^3 \to 0 \tag{1}$$

which follows from the fact that coboundary is dual to the boundary with respect to the pairing between chains and cochains. De Rham's theorem implies that the k^{th} singular cohomology and the k^{th} cohomology are isomorphic. By assumption Ω is contractible and so every closed form is a differential. Translated to cochains we have that every cocycle is a coboundary. As a result,

$$\delta b = 0 \text{ if and only if there exists } a \in C^1 \text{ such that } b = \delta a.$$

This result is fundamental to our remap algorithm. Instead of using Lagrange multipliers to enforce the divergence free constraint, or a constrained transport to advect the divergence free field, we will obtain that field by remapping its potential *a* and then applying the coboundary.

Explicit recovery of the potential

The key to the constrained interpolation remap algorithm is explicit recovery of the potential $a \in C^1$. To develop the recovery procedure let $K \in C_2$ denote a quadrilateral cell with vertices $\left\{\sigma^1_{ij}\right\}$, *i,j*=0,1 and faces $\left\{\sigma^2_F\right\}$, *F*∈(*D,U,R,L*), for the "Down", "Up", "Right" and "Left" faces. When the grid is logically Cartesian, the 2-chains can be oriented in a particularly simple manner. Specifically, we will assume that for each cell $K \in C_2$, the "horizontal" faces *U* and *D* are oriented by choosing the normal that points in the North direction, and that the "vertical" faces *L* and *R* are oriented by the normal that points in the East direction.

We identify the vertices of the cell with the edges of its three-dimensional extruded counterpart. Since chains and cochains are isomorphic, the sets $\left\{\sigma^1_{ij}\right\}$ and $\left\{\sigma^2_F\right\}$ are bases of C^1 and C^2, respectively, on *K*. As a result, on *K*, any $a \in C^1$ and $b \in C^2$ are given by the expansions

$$a = \sum_{i,j=0,1} a_{ij}\sigma^1_{ij} \text{ and } b = \sum_{F=D,U,R,L} b_F \sigma^2_F, \tag{2}$$

respectively. Considering the orientation convention for the faces of *K,* it is easy to see that the coboundary of $b \in C^2$ is given by the formula

$$\delta b = b_R + b_U - b_L - b_D \tag{3}$$

and that the coboundary of $a \in C^1$ is given by the formula

$$\delta a = a_{00}\left(\sigma_D^2 - \sigma_L^2\right) + a_{10}\left(-\sigma_R^2 - \sigma_D^2\right) + a_{01}\left(\sigma_L^2 + \sigma_U^2\right) + a_{11}\left(\sigma_R^2 - \sigma_U^2\right). \tag{4}$$

Equivalently, we can write Eq. (4) as

$$\delta a = \left(a_{00} - a_{10}\right)\sigma_D^2 + \left(a_{01} - a_{11}\right)\sigma_U^2 + \left(a_{11} - a_{10}\right)\sigma_R^2 + \left(a_{01} - a_{00}\right)\sigma_L^2. \tag{5}$$

Note that $\delta a \in C^2$ and $\delta\delta a = 0$.

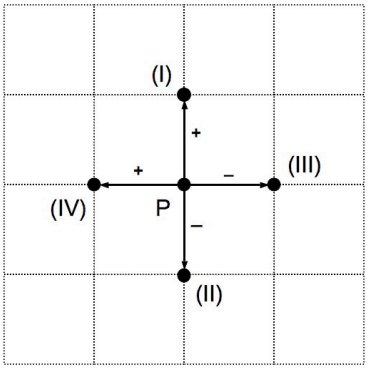

Figure 1. Recovery of the potential at four adjacent vertices.

Assume now that $b \in C^2$ is such that $\delta b = 0$. We know that *b* has a potential *a* and from the expressions for the action of the coboundary on 1 and 2-cochains in Eqs. (3) and (5) we see that $b = \delta a$ if and only if

$$b_D = \left(a_{00} - a_{10}\right); \quad b_L = \left(a_{01} - a_{00}\right); \quad b_U = \left(a_{01} - a_{11}\right); \quad b_R = \left(a_{11} - a_{10}\right). \tag{6}$$

From Eq. (6) one can determine recursively the value of the potential at any vertex (*i,j*) as follows. Assume that *a* is known at a vertex **P**. On logically Cartesian grids this vertex has exactly four neighbors, labeled by (i), (ii), (iii) and (iv); see Fig. 1. Then, from Eq. (6), it is not hard to see that if *Q* is one of these four vertices, then

$$a(Q) = a(P) + \nu b_F, \tag{7}$$

where b_F is the value of *b* associated with the face *QP* and

$$\nu = \begin{cases} 1 & \text{if } Q \text{ is (i) or (iv)} \\ -1 & \text{if } Q \text{ is (ii) or (iii)} \end{cases}. \tag{8}$$

We can use this formula to determine recursively the potential at every point *Q* on the grid by starting at an arbitrary (but fixed) vertex Q_0 and then connecting that vertex with *Q* by a 2-chain. Figure 2 shows that, in fact, potential values will be computed at every point along the indicated 2-chain. The initial value at Q_0 represents a "gauge" and selects a potential from an equivalence class of potentials that differ by a constant. This value is not important for the divergence free field and can be set to zero.

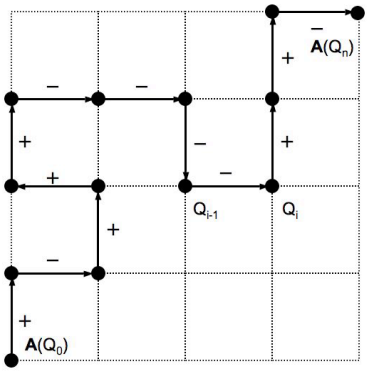

Figure 2. Recovery of the potential at vertices along a chain.

If an initial vertex and a gauge value have been fixed, the value of the recovered potential does not depend on the path between the initial vertex and the point. To see this, consider a pair of 2-chains

$$C_1 = \sum_{S_1} \nu_{S_1} \sigma^2_{S_1} \text{ and } C_2 = \sum_{S_2} \nu_{S_2} \sigma^2_{S_2} \tag{9}$$

that start and terminate at the same two endpoints and let Ω_C denote the region enclosed by them. Then, $\partial\Omega_C = C_2 - C_1$, and since $\delta b = 0$, using duality of chains and cochains, we find that

$$0 = \langle \delta b, \Omega_C \rangle = \langle b, \partial\Omega_C \rangle = \langle b, C_2 \rangle - \langle b, C_1 \rangle. \tag{10}$$

The uniqueness of *a* follows by observing that the value of the potential is given by the contraction $\langle b, C_2 \rangle$ of *b* with the chain C_2 and that according to the above $\langle b, C_2 \rangle = \langle b, C_1 \rangle$.

To summarize, given a discrete divergence free field *b* we can recover its potential by choosing a 2-chain that forms a spanning tree for the grid and then computing recursively the contraction of *b* with the subchains of that spanning tree.

Constrained Interpolation Algorithm

Using the explicit recovery procedure presented in the last section, we can now formulate the constrained interpolation remap algorithm as follows. Let $\mathcal{R}$ denote a high order *reconstruction* operator and assume that $\mathcal{I} : \mathcal{K} \to \tilde{\mathcal{K}}$ is a bounded linear *interpolation* operator between the two chain complexes. The operator $\mathcal{R}$ can be defined using a number of techniques from finite element and finite difference methods and will not be discussed here. For an example of a *patch recovery* approach, we refer to (Bochev and Shashkov, 2005). Construction of the interpolation operator for vertex-based values can be accomplished using standard C^0 Lagrange finite element basis functions. The constrained interpolation remap algorithm comprises of the following three steps.

(1). **Potential recovery**: given a discrete divergence free *b* define a spanning tree and compute *a*.

(2). **Postprocessing and optimization:**

a. define the parameterized potential by

$$a(\lambda) = \lambda a + (1-\lambda)\mathcal{R}(a)$$

where λ is a real function whose values are in [0,1].

b. compute λ_{opt} by solving the optimization problem

$$\lambda_{opt} = \arg\min \sum_{\tilde{K}\in\tilde{C}_2} \left(\|\delta a\|^2 - \|\delta \mathcal{I} a(\lambda)\|^2 \right)^2$$

(3). **Remap of *b*:** set $\tilde{a} = \mathcal{I}a(\lambda_{opt})$ and define $\tilde{b} = \delta\tilde{a}$.

The potential a determined in Step 1 is first-order accurate and may cause substantial energy dissipation in the remap. The high-order reconstruction operator is needed to reduce the loss of energy. However, using only the high-order potential $\mathcal{R}(a)$ may cause an increase in the total energy. The optimization step controls the energy by using a convex combination of a and $\mathcal{R}(a)$. The cost functional penalizes the energy difference between the original and the candidate discrete divergence free fields with respect to the cells on the "new" chain complex $\tilde{\mathcal{K}}$. To avoid solution of a global optimization problem we approximate λ_{opt} by a piecewise constant function $\lambda_{opt}(\tilde{K})$, defined by solving local optimization problems on each cell $\tilde{K}$ of the "new" complex:

$$\lambda_{opt}(\tilde{K}) = \arg\min\left(\|b\|^2_{\tilde{K}} - \left\|\delta a\left(\lambda(\tilde{K})\right)\right\|^2_{\tilde{K}} \right). \tag{11}$$

Simpler solutions can be defined by approximating λ_{opt} by a single constant, or by using a feedback control loop. For more details about these methods, we refer to (Bochev and Shashkov, 2005).

Numerical Examples

We test the constrained interpolation algorithm using a cyclic remap approach proposed in (Margolin and Shashkov, 2003). The method uses a sequence of grids parameterized by a fictitious time parameter taking values between 0 and 1, such that the first and the last grids in the sequence coincide. Therefore, cyclic remap allows to asses the cumulative effect of many remappings by comparing the initial and the final fields. In the first example the constrained interpolation algorithm is used to remap the smooth divergence-free field $\mathbf{B} = \nabla \times (\sin(2\pi x)\sin(2\pi y))$ on a sequence of 100 randomly perturbed uniform grids. Figure 3 shows the total energy of the remapped field as a function of the fictitious time. As expected, using a first-order potential is accompanied by energy loss, the high-order potential leads to energy growth, while using any one of the three energy control methods, mentioned in the last section, helps to maintain an almost constant energy throughout the remap cycle.

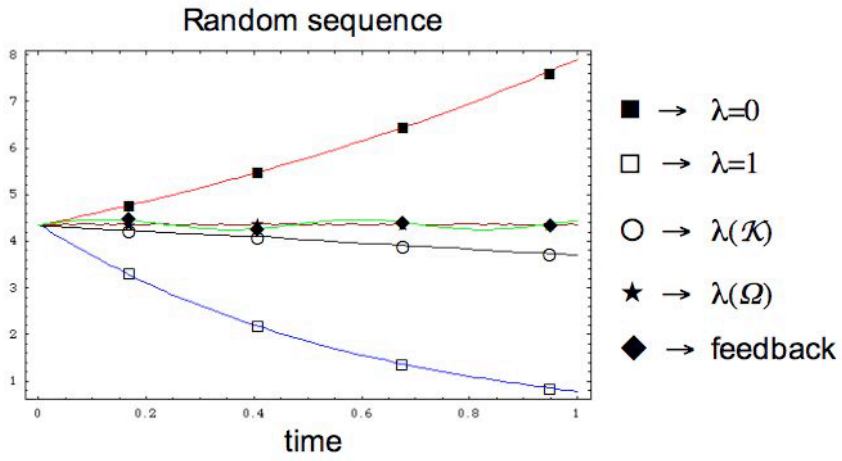

Figure 3. Energy of the remapped field for different choices of the parameter. First-order potential: λ=1, high-order potential: λ=0; and three optimization strategies.

In the second example, the algorithm is used to remap a discontinuous divergence free field on a sequence of 100 smoothly deformed uniform grids. For a precise definition of the grid sequence we refer to (Margolin and Shashkov, 2003) and (Bochev and Shashkov, 2005). The goal of this experiment is to compare performance of piecewise constant and a constant approximation of the parameter λ_{opt}. Figure 4 shows that in both cases the discontinuity is captured fairly well and is not overly smeared. However, approximation of λ_{opt} by a single constant leads to visible under and overshoots near the discontinuity. This is caused by the inability of a single control parameter to account for the local variation in the field behavior. In contrast, using a piecewise constant approximation of λ_{opt}, computed on each cell, helps to maintain an almost monotone profile of the discontinuous solution component.

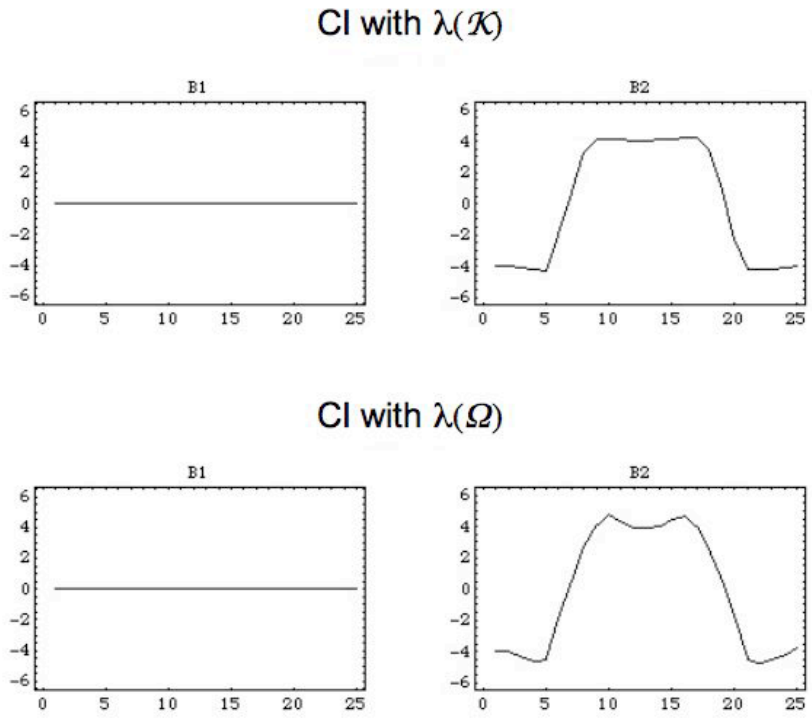

Figure 4. Comparison of a piecewise constant (top) vs. a constant (bottom) approximation for λ_{opt} and a discontinuous divergence free field.

Conclusions

We presented a remap algorithm for divergence free fields encoded by 2-cochains on a two-dimensional cell complex. The algorithm takes advantage of the existence of discrete potentials to define the remap procedure. It is applicable to a broad range of spatial discretizations that use cochain representations of vector and scalar fields. The use of interpolation instead of advection makes the algorithm appropriate for general grid configurations, including grids that have different topologies and grids that are not small perturbations if each other.

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